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# STRAIN GRADIENT CRYSTAL PLASTICITY: A CONTINUUM MECHANICS APPROACH TO MODELING MICRO-STRUCTURAL EVOLUTION

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**ABSTRACT-** In agreement with dislocation theory, recent experiments show, both quantitatively and qualitatively, how geometrically necessary dislocations (GNDs) distribute in dislocation wall and cell structures. Hence, GND density fields are highly localized with large gradients and discontinuities occurring between the cells. This behavior is not typical for strain gradient crystal plasticity models. The present study employs a higher order extension of conventional crystal plasticity theory in which the viscous slip rate is influenced by the gradients of GND densities through a back stress. A phenomenological back stress formulation is proposed, through which the effect of the GND gradient exponent can be studied. It is shown that this model can lead to more localized GND distributions.

**INTRODUCTION:** Published electron backscatter diffraction (EBSD) measurements on a face centered cubic (FCC) nickel single crystal, subject to plane strain wedge indentation, show distinct dislocation patterns (see e.g. Kysar et al. 2010). These patterns represent clear dislocation wall and cell structures, thus highly non-uniform distributions of geometrically necessary dislocations (GNDs) are present, producing discontinuities in the lattice rotations. However, existing continuum models of the micro-structural evolution tend to show a much more smoothed GND field. When the overall dimensions become comparable to the material length scale and deformation gradients become large, so called higher order strain gradient plasticity theories are needed to obtain accurate results. In the present study a non-work conjugate type theory is adopted, which is a higher order extension of conventional crystal plasticity theory. One obvious issue with modeling these experimentally observed physical phenomena, in terms of continuous field quantities, is that the evolution of dislocation structures is inherently a discrete and discontinuous process. This challenge, in particular, motivates the present study, in which the aim is to improve the accuracy of predicting micro-structural evolution using strain gradient crystal plasticity theory in continuum mechanics framework. One key to modeling the GND density distributions observed experimentally is through a back stress formulation, which is related to gradients of GND densities and influences the viscous slip rate in the adopted theory. The work presents an investigation of a phenomenological constitutive equation for the back stress based on experimental observations. Thereby, a new formulation for predicting the micro-structural evolution and plastic material response, of ductile crystalline materials, on the sub-micron level, is proposed. The influence of two key parameters on the GND density distribution is demonstrated through a parametric study.

**PROCEDURES, RESULTS AND DISCUSSION:** The present study employs a strain gradient plasticity theory within a conventional small strain elasto-viscoplastic framework, proposed by Kuroda and Tvergaard (2008). An additive decomposition of the total strain,  $\epsilon_{ij} = \epsilon_{ij}^e + \epsilon_{ij}^p$ , into an elastic part,  $\epsilon_{ij}^e$ , and a plastic part,  $\epsilon_{ij}^p$ , is used. Plastic strain is due to crystallographic slip rates,  $\dot{\gamma}^{(\alpha)}$ , on slip planes denoted  $\alpha$

$$\dot{\epsilon}_{ij}^p = \sum_{(\alpha)} \dot{\gamma}^{(\alpha)} P_{ij}^{(\alpha)}, \quad P_{ij}^{(\alpha)} = \frac{1}{2}(s_i^{(\alpha)} m_j^{(\alpha)} + s_j^{(\alpha)} m_i^{(\alpha)}) \quad (1)$$

with  $P_{ij}^{(\alpha)}$  being the Schmid orientation tensor, and  $s_i^{(\alpha)}$  and  $m_j^{(\alpha)}$  the direction of slip and the slip plane normal, respectively. Apart from the conventional stress equilibrium equation,  $\sigma_{ij,j} = 0$ , an additional set of differential equations is solved in a staggered solution scheme to obtain the GND density:

$$\frac{1}{b} \dot{\gamma}_{,i}^{(\alpha)} s_i^{(\alpha)} + \rho_{G(e)}^{(\alpha)} = 0, \quad \frac{1}{b} \dot{\gamma}_{,i}^{(\alpha)} p_i^{(\alpha)} + \rho_{G(s)}^{(\alpha)} = 0. \quad (2)$$

Here,  $\mathbf{p}^{(\alpha)} = \mathbf{s}^{(\alpha)} \times \mathbf{m}^{(\alpha)}$ ,  $b$  is the magnitude of the Burgers vector, and  $\rho_{G}^{(\alpha)}$  are GND densities on slip system  $\alpha$ . The subscripts  $(e)$  and  $(s)$  denote edge and screw components, respectively. The slip rates are given by a simple extension of the widely used visco-plastic power law slip rate relation

$$\dot{\gamma}^{(\alpha)} = \dot{\gamma}_0 \text{sgn} \left( \tau^{(\alpha)} - \tau_b^{(\alpha)} \right) \left( \frac{|\tau^{(\alpha)} - \tau_b^{(\alpha)}|}{g^{(\alpha)}} \right)^{1/m}, \quad (3)$$

where  $\tau$  is the Schmid stress taken as the projection of the macroscopic Cauchy stress tensor onto the slip plane,  $\tau_b$  is a back stress,  $m$  is the rate hardening exponent, and  $g$  is the slip resistance. The gradient energy is often taken to be of a quadratic nature of the form

$$\psi_G = \frac{1}{2} \tau_0 L^2 \left( s_i^{(\alpha)} \dot{\gamma}_{,i}^{(\alpha)} \right)^2, \quad (4)$$

where  $L$  is a material length scale parameter and  $\tau_0$  is the initial critical resolved shear stress. This is, however, mostly for mathematical convenience rather than based on physical arguments. Relating the back stress to the gradient energy as in Kuroda and Tvergaard (2008), Eq. (4) leads to

$$\tau_b^{(\alpha)} = -\tau_0 L^2 s_i^{(\alpha)} s_j^{(\alpha)} \dot{\gamma}_{,ij}^{(\alpha)} = b \tau_0 L^2 s_i^{(\alpha)} \rho_{G(e),i}^{(\alpha)}, \quad (5)$$

in which case the theory coincides with the work conjugate theory of Gurtin (2002). In order to explore the effect of the relationship between the back stress and the gradients of GND density, we construct a phenomenological back stress power law in the light of the experimental observations. Thus, we introduce a dependence on the gradients of GND density to the power of a parameter  $\mu$ , taking a value between zero and one:

$$\tau_b^{(\alpha)} = \text{sgn} \left( s_i^{(\alpha)} \rho_{G(e),i}^{(\alpha)} \right) b^\mu \tau_T^{1-\mu} \tau_0^\mu L^{2\mu} \left| s_i^{(\alpha)} \rho_{G(e),i}^{(\alpha)} \right|^\mu, \quad \text{for } \tau_b^{(\alpha)} > \tau_T, \quad (6)$$

with  $\tau_T$  being a transition back stress parameter. At the limit of  $\mu = 0$ , the function initially has an infinite slope. To avoid the difficulties tied to low values of  $\mu$ , the back stress is assumed to evolve according to Eq. (5) until  $\tau_b^{(\alpha)} > \tau_T$ . With  $\mu = 0$ , Eq. (6) corresponds to a blunt cut-off of the back stress at  $\tau_b^{(\alpha)} = \tau_T$ . For  $\mu = 1$ , Eq. (5) and (6) are identical, corresponding to a quadratic gradient energy throughout. The theory is applied to a constrained single slip pure shear problem, with height  $H$ , Young's modulus  $E = 130$  MPa, Poisson's ratio  $\nu = 0.3$ ,  $\tau_0 = 50$  MPa,  $\tau_T/\tau_0 = 0.12$ , and  $L/H = 0.3$ . The slip system is perpendicular to the shearing direction. Fig. 1 shows the GND density profile for different values of the rate exponent  $m$ , with  $\mu = 1$  (Fig. 1a) and with  $\mu = 0.4$  (Fig. 1b). As  $\mu$  becomes smaller than unity, the GND density evolves more intensely at the boundaries, resulting in more pronounced dislocation "wall"-structures forming. Particularly for the higher values of  $m$  the effect of  $\mu$  is clear. This micro-structural response bears closer resemblance to what is observed in experimental studies.

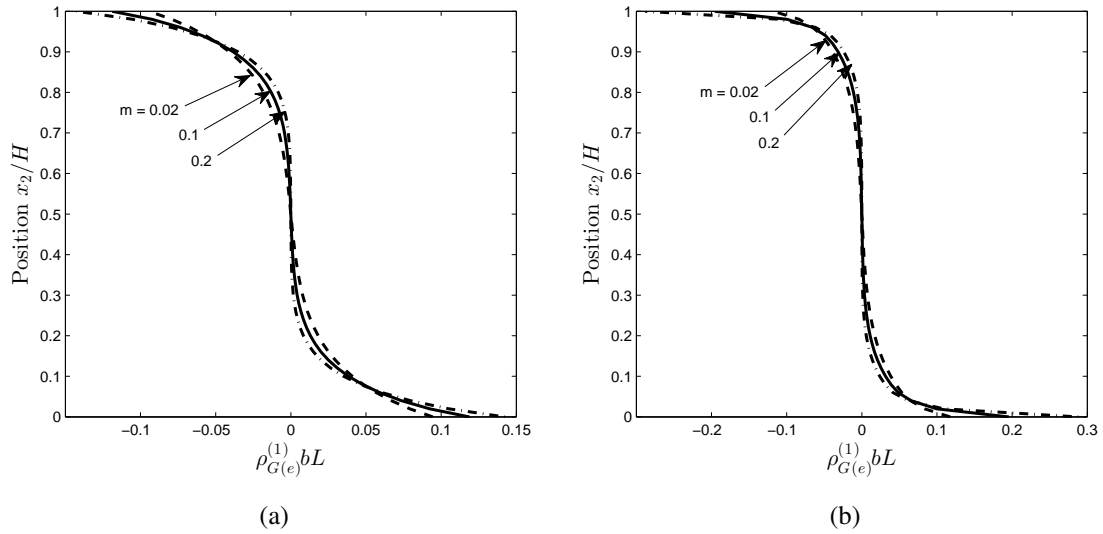


Figure 1: Normalized GND density profile for single slip simple shear of periodic material domain, for different values of the rate exponent  $m$ . (a) with  $\mu = 1$ , and (b) with  $\mu = 0.4$ .

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